Atmos. Chem. Phys. Discuss., 11, C10423–C10425, 2011
www.atmos-chem-phys-discuss.net/11/C10423/2011/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "ANISORROPIA: the adjoint of the aerosol thermodynamic model ISORROPIA" *by* S. L. Capps et al.

D. Dabdub

ddabdub@uci.edu

Received and published: 15 October 2011

Manuscript Number: ACPD-11-23469-2011

Title: ANISORROPIA: the adjoint of the aerosol thermodynamic model ISORROPIA

The paper presents the adjoint of ISORROPIA, a thermodynamic model to simulate inorganic aerosols that is implemented in several chemical transport models (CTM). Model adjoints have been available for gas-phase species for many of the CTM that employ ISORROPIA, and hence, an adjoint for aerosol species would complement current model capabilities in order to determine model sensitivity to model inputs and parameters.

Reviews by Jim Kelly (Sept 19, 2011) and an anonymous referee (Sept 26, 2011) al-

ready suggested a comprehensive list of revisions needed to be addressed before the paper can be accepted for publication. Overall, I agree with their suggestions and evaluation. Namely, this is an important first step in the development of the adjoint of ISORROPIA. However, some important issues need to be addressed before publication.

In order to avoid repetition, this review adds new specific comments and emphasizes further aspects that would help clarify the manuscript.

General Comments

One point that stands out is the issue with convergence. As Jim Kelly suggested, a more in depth analysis of the cases in which the model did not converge would help the readers understand the applicability of the model. For instance, discussion in section 4.1 presents ternary diagrams based on a range of concentrations for total NH3, H2SO4 and HNO3. Did the entire concentration space presented in those diagrams converge? It would be quite informative to provide some insights on whether there are some of the 10 regimes assumed in ISORROPIA more conducive to problems with convergence. In addition, the criteria for convergence are not clear. Is the 30% rate for non-convergence sensitive to those criteria? Also, how would those criteria affect computational expenses?

Another point is the lack of discussion on implementation of ANISORRPIA in a CTM. The last statement in the abstract is misleading. Even if it might be true, it is not directly addressed in the paper. In addition, the last statement in section 1 does not correspond with the work presented in the manuscript.

Finally, I strongly second Jim Kelly's comment on section 2.1. It includes an extensive description of mathematical background that seems disconnected from the rest of the paper.

Specific Comments

In page 23481, line 7, the use of [X] is confusing as there is not any X in the preceding equation. The same goes for page 23487, line 16.

In page 23484, lines 20-21: There is no comment on how ANISORROPIA performs at low temperatures (268-288 K) compared to higher temperatures. This is important since many high PM events occur in winter.

The axes in Figures 6 and 8 are misleading, as the other reviewers pointed out. It seems that the axes titles correspond to the values with the same alignment, but the reader cannot be sure that the values in the axes are correctly laid out.

In figure 6, for 90% relative humidity, there are some ripples and curves that are difficult to explain. Is this related to convergence issues? Or is this related to the treatment of 10 different regimes? In this last case, would it add value to the discussion to add graphically the boundaries of the possible regimes existing in that ternary system?

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 23469, 2011.